

Localization of non-relativistic particles

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Abstract

This paper is a contribution to the problem of particle localization in non-relativistic Quantum Mechanics. Our main results will be (1) to formulate the problem of localization in terms of invariant subspaces of the Hilbert space, and (2) to show that the rigged Hilbert space incorporates particle localization in a natural manner.

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1 Introduction

In Quantum Mechanics courses, we are taught that the concept of trajectory does not make any sense in the quantum realm. We are also taught that the solutions to the Schrödinger equation are not supposed to be interpreted as real waves, but rather as probability amplitudes—in Quantum Mechanics, what is “waving” is probability. We are therefore encouraged to picture particles not as point-like entities, but rather as sort of clouds of probability. This picture is reinforced by, for example, drawings of orbitals of the Hydrogen atom, or by animations of wave packets impinging upon a barrier.

We nevertheless like to think that when performing an experiment in the lab with, say, atoms, the wave functions that describe the atoms are localized in the lab. We definitely don’t picture the atomic wave functions spreading all around space. Instead, we naively expect that we prepare clouds of probability that are localized in the lab, and that those clouds remain localized in the lab during the experiment. In this paper, we discuss to what extent such naive expectation holds in non-relativistic Quantum Mechanics.

Mathematically, the problem of localization can be formulated as follows. Given a wave function f that is localized at $t = 0$, does f remain localized as time goes on? We shall see that such question is best formulated as the invariance of subspaces of the Hilbert space under the time evolution group. Particle localization can therefore be reduced to the study of invariant subspaces of the Hilbert space under time evolution.

The structure of this paper is as follows. In Sec. 2, we discuss three types of localization (compact-support, polynomial and exponential) and formulate them as the invariance of certain subspaces of the Hilbert space under time evolution. In Sec. 3,

we discuss the compact-support localization. Although it is well known that compact-support localization is not possible, we anyway discuss it, for the sake of completeness and for the sake of comparison with polynomial and exponential localizations. In Sec. 4, we discuss the theorems that are most relevant to polynomial localization. In Sec. 5, we discuss exponential localization. In Sec. 6, we explain how localization is built into a rigged Hilbert space. Finally, in Sec. 7, we state our conclusions.

Our discussion will be elementary and, unfortunately, we shall not be able to prove whether exponential localization holds, which is the remaining challenge of non-relativistic particle localization.

2 Three types of localization

Quantitatively, the localization of a particle is characterized by the rate at which its wave function falls off outside the region where the particle is supposed to be localized. There are many ways to characterize such falloff. The three most important falloff regimes, which are also the ones we are concerned with in this paper, are the compact-support, the polynomial and the exponential regimes (see Fig. 1):

$$\text{comp. supp.} \prec \cdots \prec \overbrace{e^{-x^n} \prec \cdots \prec e^{-x^2} \prec e^{-x}}^{\text{exponential regime}} \prec \cdots \prec \overbrace{\frac{1}{x^n} \prec \cdots \prec \frac{1}{x^2} \prec \frac{1}{x}}^{\text{polynomial regime}}, \quad (2.1)$$

where $a \prec b$ indicates that the falloff “ a ” is stronger than the falloff “ b .” Within each regime, one can differentiate several sub-regimes. For example, in the polynomial regime, one can have $1/x$ falloff, $1/x^2$ falloff, and so on.

In functional-analysis terms, the localization of particles can be formulated by constructing subspaces of the Hilbert space whose wave functions satisfy the desired localization conditions. Thus, for compact-support localization, we construct the space $\Phi_{\text{c.s.}}$ of functions f that vanish beyond a finite distance $R_f > 0$:

$$\Phi_{\text{c.s.}} = \{f \in L^2 \mid |f(x)| = 0 \text{ for } |x| > R_f; \text{ and additional properties}\}, \quad (2.2)$$

where in “additional properties” we include other extra properties that the wave functions may have to satisfy (e.g., differentiability). For polynomial localization of order n , we define the space of wave functions that fall off faster than x^n :

$$\Phi_{\text{pol}} = \{f \in L^2 \mid |x^n f(x)| \rightarrow 0 \text{ when } |x| \rightarrow \infty; \text{ and additional properties}\}. \quad (2.3)$$

We can also demand polynomial localization to all orders, as with the Schwartz space. For exponential localization of order n , we define the space of wave functions that fall off faster than $e^{|x|^n}$:

$$\Phi_{\text{exp}} = \{f \in L^2 \mid |e^{|x|^n} f(x)| \rightarrow 0 \text{ when } |x| \rightarrow \infty; \text{ and additional properties}\}. \quad (2.4)$$

We note that the “additional properties” of Eqs. (2.2)-(2.4) may be necessary to ensure localization. For example, we shall see that polynomial localization does not hold unless additional properties are demanded from the wave functions.

Now, a particle is localized in a compact-support, polynomial or exponential sense when the spaces $\Phi_{\text{c.s.}}$, Φ_{pol} or Φ_{exp} remain invariant under the time evolution group:

$$e^{-iHt}\Phi_{\text{c.s.}} \subset \Phi_{\text{c.s.}} , \quad (2.5)$$

$$e^{-iHt}\Phi_{\text{pol}} \subset \Phi_{\text{pol}} , \quad (2.6)$$

$$e^{-iHt}\Phi_{\text{exp}} \subset \Phi_{\text{exp}} . \quad (2.7)$$

Therefore, finding out whether a particle can be localized in a compact-support, polynomial or exponential sense is equivalent to finding out whether the invariances (2.5)-(2.7) hold for a given Hamiltonian. In the following three sections, we list some of the results that guarantee or forbid such invariances.

3 Compact-support localization

It is well known that if a non-relativistic particle is initially confined to a finite region of space, then it immediately develops infinite tails, as one could already expect from the lack of an upper limit for the propagation speed in non-relativistic Quantum Mechanics. Thus, compact support localization is impossible,

$$e^{-iHt}\Phi_{\text{c.s.}} \not\subset \Phi_{\text{c.s.}} . \quad (3.1)$$

The free Hamiltonian H_0 provides a transparent way of seeing why a particle initially localized in a finite region immediately spreads throughout all space. One simply has to calculate the time evolution of a wave packet φ from the well-known expression for the free propagator ($\hbar = 1$):

$$\varphi(\mathbf{x}; t) = e^{-iH_0t}\varphi(\mathbf{x}) = \left(\frac{m}{2\pi it}\right)^{3/2} \int d^3\mathbf{y} e^{im|\mathbf{x}-\mathbf{y}|^2/(2t)}\varphi(\mathbf{y}) . \quad (3.2)$$

The wave function $\varphi(\mathbf{x}; t)$ is the superposition of the amplitudes produced by the waves emitted at $t = 0$ from all points \mathbf{y} in space. Thus, even when $\varphi(\mathbf{x})$ is zero outside a finite region V_0 at $t = 0$, at any other time, $\varphi(\mathbf{x}; t)$ will be non-zero for all \mathbf{x} , because the free propagator “connects” any point \mathbf{x} in space with those in the region V_0 .

An extreme case of compact-support localization occurs when the wave function is completely supported at a point \mathbf{x}_0 of space, that is, when the initial wave function is the delta function $\delta(\mathbf{x} - \mathbf{x}_0)$. For the free case, the time evolution of the delta function is given by

$$e^{-iH_0t}\delta(\mathbf{x} - \mathbf{x}_0) = \left(\frac{m}{2\pi it}\right)^{3/2} \int d^3\mathbf{y} e^{im|\mathbf{x}-\mathbf{y}|^2/(2t)}\delta(\mathbf{y} - \mathbf{x}_0) = \left(\frac{m}{2\pi it}\right)^{3/2} e^{im|\mathbf{x}-\mathbf{x}_0|^2/(2t)} . \quad (3.3)$$

Thus, if a free particle is initially localized at \mathbf{x}_0 , then it instantaneously develops sinusoidal tails all around space.

A theorem by Hegerfeldt [1, 2] (see also [3, 4]) traces the impossibility of compact-support localization to the semiboundedness of the Hamiltonian. More precisely, if at $t = 0$ the wave function is compactly supported in a region V_0 , and if the Hamiltonian that drives the time evolution is bounded from below, then

- (i) either the wave function remains compactly supported in V_0 ,
- (ii) or the wave function instantaneously develops “tails” that reach all regions of space. The spread is all over space, except for “holes” which, if they exist, will persist for all times.

In most cases, possibility (ii) applies. In some cases, however, possibility (i) applies. For example, the following potential (see Fig. 2) is able to trap particles in a finite region of space:

$$V(x) = \begin{cases} 0 & -\infty < x < a_1 & \text{region I} \\ \infty & a_1 < x < a_2 & \text{region II} \\ 0 & a_2 < x < a_3 & \text{region III} \\ \infty & a_3 < x < a_4 & \text{region IV} \\ 0 & a_4 < x < \infty & \text{region V.} \end{cases} \quad (3.4)$$

We simply have to throw the particle into region III, where it will remain forever. This potential also illustrates the possibility of “holes.” If we throw the particle in the regions I or V, then region III will remain as a “hole.”

We recall that even bound states are in general not localized in a finite region of space. For example, the bound states of the Hydrogen atom fall off like an exponential multiplied by a Laguerre polynomial, and the bound states of the Harmonic oscillator fall off like a Gaussian multiplied by a Hermite polynomial.

Since compact-support localization is in general not possible, the question now is whether the exponential and the polynomial localizations are possible, that is, whether Φ_{pol} and Φ_{exp} are invariant under the time evolution group.

4 Polynomial localization

Several theorems, especially those by Hunziker [5] and by Radin and Simon [6], guarantee that polynomial localization is possible when the potential is “reasonable.” By “reasonable” we mean that there should exist an $a < 1$ and a $b < \infty$ such that

$$\|Vf\| \leq a\|H_0f\| + b\|f\|; \quad (4.1)$$

that is, V can be seen as a small perturbation to the kinetic energy, in the sense of Kato [7]. For such potentials, we can find appropriate spaces Φ_{pol} that incorporate some type of polynomial localization and that remain invariant under the time evolution group:

$$e^{-iHt}\Phi_{\text{pol}} \subset \Phi_{\text{pol}}. \quad (4.2)$$

In order to state Hunziker’s theorem, we need first some definitions: $\mathbf{x}^n \equiv x_1^{n_1}x_2^{n_2}x_3^{n_3}$, n being the multi-index (n_1, n_2, n_3) with n_j integer, $n_j \geq 0$; $|n| = \sum_i n_i$; $k \leq n$ means $k_i \leq n_i$ for $i = 1, 2, 3$. For any multi-index n , \mathbf{x}^n also denotes the operator multiplication by the function \mathbf{x}^n . For any multi-index n , we define a linear subset D_n of $L^2(\mathbb{R}^3)$ and a norm $\|\cdot\|_n$ on D_n by

$$D_n \equiv \bigcap_{\substack{k \leq n \\ m \leq |n| - |k|}} \mathcal{D}(\mathbf{x}^k H^m), \quad (4.3)$$

$$\|f\|_n \equiv \sup_{\substack{k \leq n \\ m \leq |n|-|k|}} \|\mathbf{x}^k H^m f\|, \quad (4.4)$$

where $\mathcal{D}(\mathbf{x}^k H^m)$ denotes the domain of the operator $\mathbf{x}^k H^m$, and m denotes an integer greater than or equal to 0.

Theorem 1 (Hunziker) *Under the assumption of Eq. (4.1), the following holds for any multi-index n :*

(a) D_n is invariant under the time evolution group:

$$e^{-iHt} D_n \subset D_n. \quad (4.5)$$

(b) For any $f \in D_n$, $e^{-iHt} f$ is continuous in t in the sense of the norm $\|\cdot\|_n$, and there exists a constant c_n such that

$$\|e^{-iHt} f\|_n \leq c_n (1 + |t|)^{|n|} \|f\|_n. \quad (4.6)$$

Since the norms of Eq. (4.4) imply that the elements of D_n fall off faster than $1/\mathbf{x}^n$ at infinity, Theorem 1 ensures the $1/\mathbf{x}^n$ -localization of the elements of D_n .

Theorem 1 is valid not only in three but in any dimension, a result we shall take advantage of in Sec. 6. In addition, when the potential is a C^∞ -function with bounded derivatives, Theorem 1 implies that the Schwartz space is invariant under time evolution:

Corollary (Hunziker) *If $V(\mathbf{x})$ is a bounded C^∞ -function on \mathbb{R}^3 with bounded derivatives, then $\mathcal{S}(\mathbb{R}^3)$ is invariant under the unitary group e^{-iHt} and the mapping $(\varphi, t) \rightarrow e^{-iHt} \varphi$ of $\mathcal{S}(\mathbb{R}^3) \times \mathbb{R}$ onto $\mathcal{S}(\mathbb{R}^3)$ is continuous (in the sense of the conventional topology of $\mathcal{S}(\mathbb{R}^3)$).*

Therefore, when a particle is initially localized better than any polynomial of \mathbf{x} , and when the potential that drives the evolution of the particle is a C^∞ -function, then the particle remains localized better than any polynomial of \mathbf{x} as time goes on.

A result by Radin and Simon resembles and complements Hunziker's theorem:

Theorem 2 (Radin-Simon) *Let V obey Eq. (4.1). Let*

$$S_1 \equiv \{f \in L^2 \mid |\mathbf{x}|f \in L^2, |P|f \in L^2\}, \quad (4.7)$$

$$S_2 \equiv \{f \in L^2 \mid \mathbf{x}^2 f \in L^2, P^2 f \in L^2\}, \quad (4.8)$$

and respectively equip these spaces with the norms

$$\|f\|_1 \equiv (\|f\|^2 + \||\mathbf{x}|f\|^2 + \||P|f\|^2)^{1/2}, \quad (4.9)$$

$$\|f\|_2 \equiv (\|f\|^2 + \||\mathbf{x}|^2 f\|^2 + \|P^2 f\|^2)^{1/2}. \quad (4.10)$$

Then S_1 and S_2 remain invariant under e^{-iHt} ,

$$e^{-iHt}S_1 \subset S_1, \quad (4.11)$$

$$e^{-iHt}S_2 \subset S_2, \quad (4.12)$$

and

$$\|e^{-iHt}f\|_1 \leq (c + d|t|) \|f\|_1, \quad (4.13)$$

$$\|e^{-iHt}f\|_2 \leq (c' + d't^2) \|f\|_1, \quad (4.14)$$

where c, d, c', d' are constants.

At infinity, the elements of S_1 and S_2 fall off faster than $1/|\mathbf{x}|$ and $1/\mathbf{x}^2$, respectively. Thus, Theorem 2 ensures the $1/|\mathbf{x}|$ - and the $1/\mathbf{x}^2$ -localization of the elements of S_1 and S_2 , respectively.

Theorem 2 can be extended to higher polynomial falloffs; more precisely, under the conditions of Theorem 2, the space

$$S_n = \{f \in L^2 \mid |\mathbf{x}|^n f \in L^2, |P|^n f \in L^2\} \quad (4.15)$$

is invariant under e^{-iHt} , for each positive n [8].

It is interesting that the falloff properties of a wave function f are not preserved under e^{-iHt} when f has some singularities [8]. Thus, a wave function f that is polynomially localized at $t = 0$ will remain polynomially localized only if f is smooth enough. Hence, the space Φ_{pol} of Eq. (2.3) always needs some “additional properties” in order to remain invariant under e^{-iHt} .

There are other results on polynomial localization, all of them stating basically that polynomial localization is possible when the wave function is smooth enough. We shall not list all those results here; instead, we shall move on to the problem of exponential localization.

5 Exponential localization

Contrary to polynomial localization, there doesn't seem to exist accurate results that guarantee exponential localization of non-relativistic particles. Some basic results, however, indicate that exponential localization is possible.

It is well known that a Gaussian wave packet remains Gaussian under free time evolution. Thus, if the wave function of a free particle has Gaussian tails at $t = 0$, and if that wave function is smooth enough, we expect that those Gaussian tails will remain so as time goes on.

If the time evolution is driven by a Hamiltonian $H = H_0 + V$, we expect that Gaussian tails remain so as time goes on, provided that the potential V is a small perturbation to H_0 .

In a scattering system, far from the potential region, the time evolution is essentially governed by the free Hamiltonian. Thus, Gaussian tails should be preserved in scattering processes.

We therefore expect that for reasonable potentials and for smooth wave functions, exponential localization is possible. However, the precise statements (that is, the analogs of Theorems 1 and 2) on exponential localization are still lacking.

To finish this section, we note that Bialynicki-Birula has shown that the exponential localization of photons is possible [9] (see also Ref. [10]).

6 The rigged Hilbert space and localization

The rigged Hilbert space is emerging as the natural mathematical setting for quantum mechanical continuous and resonance spectra. Surprisingly enough, the rigged Hilbert space of a system tells us a great deal about the localization properties of that system.

6.1 The rigged Hilbert space and polynomial localization

A quantum mechanical system is generally described by an algebra \mathcal{A} of observables. These observables are defined as self-adjoint operators on a Hilbert space \mathcal{H} . More often than not, those operators are unbounded and have continuous spectrum, the reason for which one needs to construct the following rigged Hilbert spaces:

$$\Phi_{\text{pol}} \subset \mathcal{H} \subset \Phi'_{\text{pol}}, \quad (6.1)$$

$$\Phi_{\text{pol}} \subset \mathcal{H} \subset \Phi^{\times}_{\text{pol}}. \quad (6.2)$$

Here, Φ_{pol} is the maximal invariant subspace of the algebra \mathcal{A} , and Φ'_{pol} and $\Phi^{\times}_{\text{pol}}$ are respectively the dual and the antidual spaces of Φ_{pol} . The space Φ_{pol} is the largest subspace of the Hilbert space that remains invariant under the action of the observables of the algebra. The spaces Φ'_{pol} and $\Phi^{\times}_{\text{pol}}$ respectively contain the bras and the kets of the observables [11, 12, 13].

In order to see how the rigged Hilbert spaces (6.1)-(6.2) incorporate polynomial localization, we shall first consider the example of a spinless particle impinging on a rectangular barrier potential [11, 12]. For this system, the algebra of observables is generated by the position, the momentum and the energy operators:

$$Qf(x) = xf(x), \quad (6.3)$$

$$Pf(x) = -i\frac{d}{dx}f(x), \quad (6.4)$$

$$Hf(x) = -\frac{1}{2m}\frac{d^2}{dx^2}f(x) + V(x)f(x), \quad (6.5)$$

where

$$V(x) = \begin{cases} 0 & -\infty < x < a \\ V_0 & a < x < b \\ 0 & b < x < \infty \end{cases} \quad (6.6)$$

is the one-dimensional rectangular barrier potential. The maximal invariant subspace of this algebra is given by a Schwartz-like space of test functions [12], which we denote

by $\mathcal{S}(\mathbb{R}-\{a, b\})$. This space can be written as

$$\mathcal{S}(\mathbb{R}-\{a, b\}) = \bigcap_{n=0}^{\infty} D_n, \quad (6.7)$$

with D_n given by Eq. (4.3). The potential (6.6) satisfies Kato's condition (4.1), because

$$\|Vf\| \leq V_0 \|f\|. \quad (6.8)$$

We are therefore allowed to apply Theorem 1. Since by Theorem 1 each D_n is invariant under e^{-iHt} , so is $\mathcal{S}(\mathbb{R}-\{a, b\})$,

$$e^{-iHt}\mathcal{S}(\mathbb{R}-\{a, b\}) \subset \mathcal{S}(\mathbb{R}-\{a, b\}). \quad (6.9)$$

This invariance, together with the polynomial falloff of the elements of $\mathcal{S}(\mathbb{R}-\{a, b\})$, ensures the polynomial localization of the elements of $\mathcal{S}(\mathbb{R}-\{a, b\})$.

From the above simple example, we can draw quite general conclusions. In general, the algebra of a non-relativistic system will always contain the position, the momentum and the energy operators. Hence, the elements of the maximal invariant subspace of the algebra, which is the space Φ_{pol} of the rigged Hilbert spaces (6.1)-(6.2), must fall off faster than any power of the position coordinate. Since for a large class of systems Hunziker's theorem ensures the invariance of Φ_{pol} under e^{-iHt} , the elements of Φ_{pol} will in general be localized better than any polynomial.

It is important to note that the rigged Hilbert spaces (6.1)-(6.2) arise from properties of the algebra of the system (Φ_{pol} is the maximal invariant subspace of the algebra). Therefore, the polynomial localization built into those rigged Hilbert spaces, rather than being imposed by hand, arises from properties of the system.

6.2 The rigged Hilbert space and exponential localization

Quantum mechanical resonances are described by the Gamow states, see e.g. [13, 14]. In the position representation, these states blow up exponentially at infinity. In order to control such exponential blow-up, we need a space Φ_{exp} of test functions that fall off faster than real exponentials [15, 13]. The space Φ_{exp} then yields two rigged Hilbert spaces in a natural way:

$$\Phi_{\text{exp}} \subset \mathcal{H} \subset \Phi'_{\text{exp}}, \quad (6.10)$$

$$\Phi_{\text{exp}} \subset \mathcal{H} \subset \Phi^{\times}_{\text{exp}}. \quad (6.11)$$

Here, Φ'_{exp} and $\Phi^{\times}_{\text{exp}}$ are respectively the dual and the antidual spaces of Φ_{exp} . The space Φ_{exp} is the largest subspace of the Hilbert space that remains invariant under the action of the observables of the algebra and whose elements fall off faster than any real exponential. The space Φ'_{exp} contains the Gamow bras, whereas the space $\Phi^{\times}_{\text{exp}}$ contains the Gamow kets.

The space Φ_{exp} must be invariant under e^{-iHt} , since such invariance is needed in the definition of the time evolution of the Gamow states. Thus, the elements of Φ_{exp} must be exponentially localized.

It is important to realize that the Gamow states are properties of the Hamiltonian, and therefore so are the rigged Hilbert spaces (6.10)-(6.11). Hence, the exponential localization built into those rigged Hilbert spaces, rather than being imposed by hand, arises from properties of the system.

We note, however, that a satisfactory Φ_{exp} has not yet been constructed for specific, simple examples. There are some proposals, though. For instance, Parravicini *et al.* [16] have proposed the space of infinitely differentiable functions with compact support on the positive real line, $C_0^\infty(0, \infty)$, as the space Φ_{exp} . But we saw in Sec. 3 that $C_0^\infty(0, \infty)$ is not invariant under e^{-iHt} for (almost) any t and any Hamiltonian, and therefore $C_0^\infty(0, \infty)$ is inappropriate as space of test functions for the Gamow states.

7 Conclusions

We have seen that the problem of localization is best formulated as the invariance of subspaces of the Hilbert space under the time evolution group. We have also seen that compact-support localization is not possible, that polynomial localization is possible, and that exponential localization is desirable and likely to be possible. Thus, in principle, we are not able to confine the wave packet of a particle to a finite region of space, although we can make the tails of the wave function fall off faster than polynomials and (probably) exponentials.

We have also seen that the rigged Hilbert space of a system incorporates localization in a natural way. The maximal invariant subspace of an algebra will in general entail polynomial localization, and the space of test functions for the Gamow states will in general entail exponential localization.

So, what about our naive expectation that the wave function of our atoms remains localized in the lab? Do those wave functions actually spread all around space, albeit with polynomial or exponential tails? In principle, of course, the tails of the wave packets reach infinity. In practice, however, such infinity is certainly within the boundaries of the lab.

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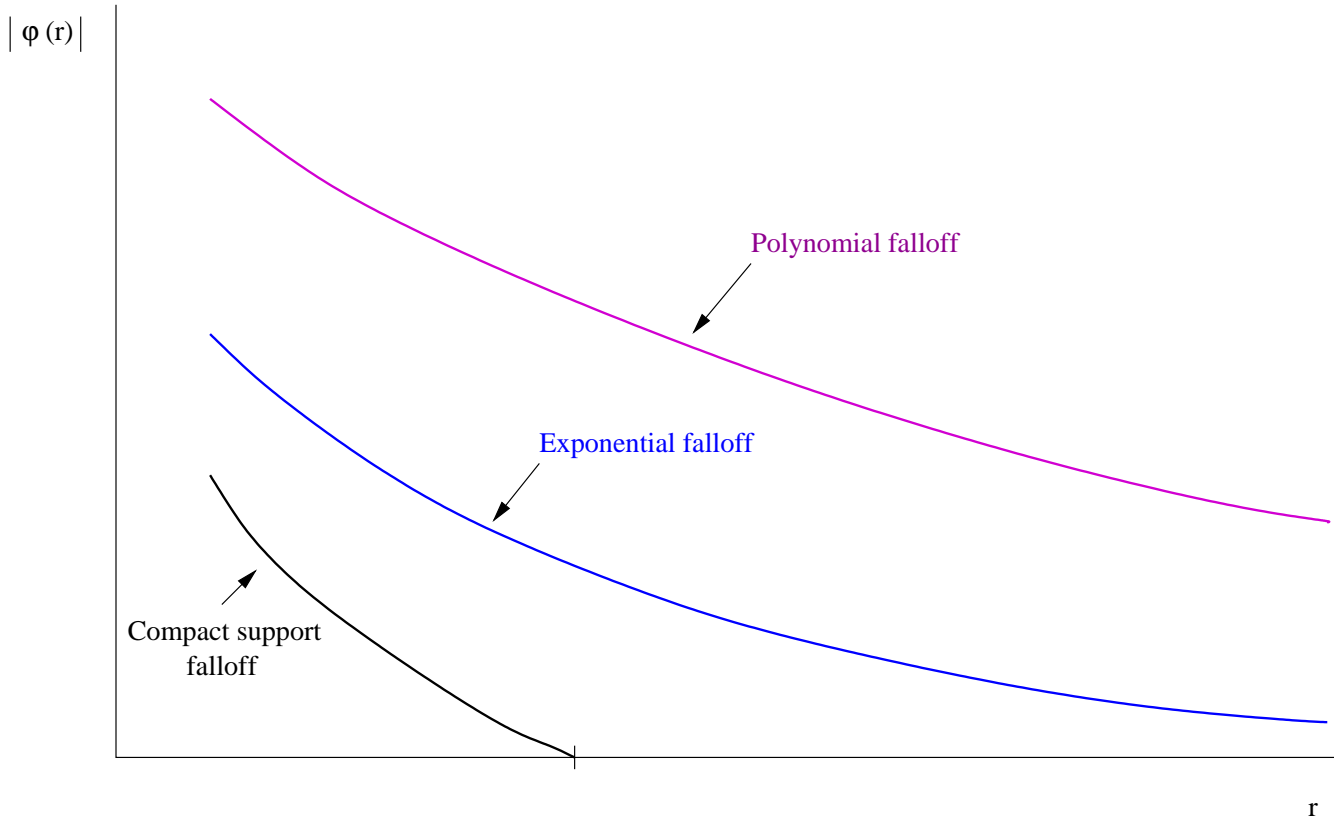


Figure 1: Schematic representation of the three regimes of particle localization.

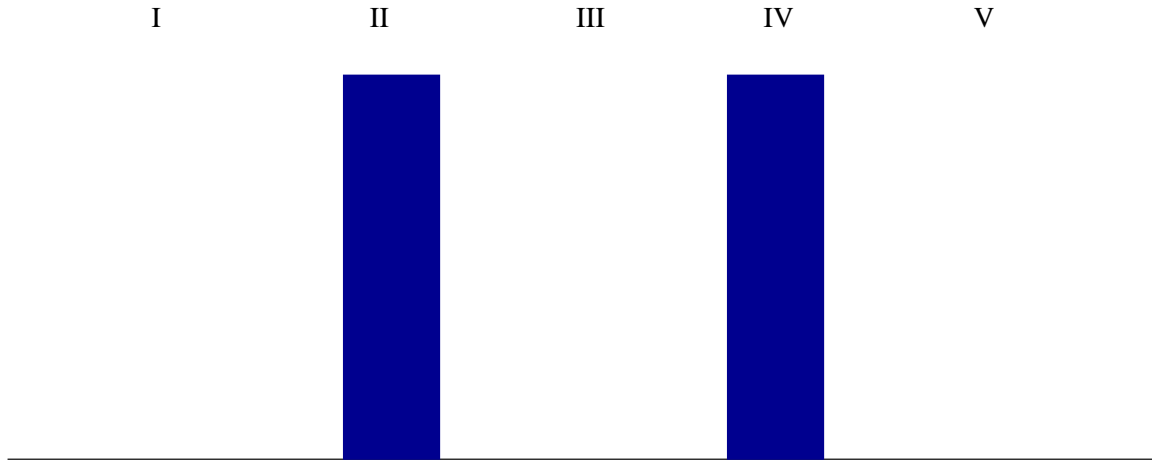


Figure 2: The potential of Eq. (3.4).